Title of Invention: Aromatic Oxyphenyl and Aromatic Sulfanylphenyl Derivatives

Inventors (please provide full names): Graeme Smith, Gitte Mikkelsen, Kim Andersen, Daniel Greve & Jørgen Eskildsen

Earliest Priority Date: 4/30/03

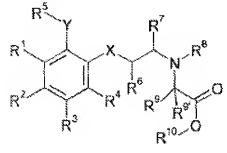
Search Topic:
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent number) along with the appropriate serial number.

Please search claim 1. Thank you!

The following listing of claims replaces all prior listings of claims presented in the application.

1. (Previously presented) A compound of the formula I



wherein

X is O, S or $CR^{11}R^{12}$, wherein R^{11} and R^{12} are each independently H or C_{1-6} alkyl;

Y is O or S;

R^1, R^2, R^3 and R^4 are each independently hydrogen; halogen; cyano; nitro; C_{1-6}-alk(en/yn)yl; C_{1-6}-alk(en/yn)yloxy; C_{1-6}-alk(en/yn)ylsulfanyl; hydroxy; hydroxy-C_{1-6}-alk(en/yn)yl; halo-C_{1-6}-alk(en/yn)yl; halo-C_{1-6}-alk(en/yn)yloxy; C_{3-8}-cycloalk(en)yl; C_{3-8}-cycloalk(en)yl-C_{1-6}-alk(en/yn)yl; acyl; C_{1-6}-alk(en/yn)yloxycarbonyl; C_{1-6}-alk(en/yn)ylsulfonyl; aryl optionally substituted with a halogen, cyano, nitro, C_{1-6}-alk(en/yn)yl, C_{1-6}-alk(en/yn)yloxy, C_{1-6}-alk(en/yn)ylsulfanyl, hydroxy, hydroxy-C_{1-6}-alk(en/yn)yl, halo-C_{1-6}-alk(en/yn)yl, halo-C_{1-6}-alk(en/yn)yloxy, C_{3-8}-cycloalk(en)yl, C_{3-8}-cycloalk(en)yl-C_{1-6}-alk(en/yn)yl, acyl, C_{1-6}-alk(en/yn)yloxycarbonyl or C_{1-6}-alk(en/yn)ylsulfonyl; monocyclic heteroaryl optionally substituted with a halogen, cyano, nitro, C_{1-6}-alk(en/yn)yl, C_{1-6}-alk(en/yn)yloxy, C_{1-6}-alk(en/yn)ylsulfanyl, hydroxy, hydroxy-C_{1-6}-alk(en/yn)yl, halo-C_{1-6}-alk(en/yn)yl, halo-C_{1-6}-alk(en/yn)yloxy, C_{3-8}-cycloalk(en)yl, C_{3-8}-cycloalk(en)yl-C_{1-6}-alk(en/yn)yl, acyl, C_{1-6}-

******* INVENTOR RESULTS *******

```
=> d his l23

     (FILE 'HCAPLUS' ENTERED AT 13:11:11 ON 26 MAR 2009)
L23            2 S ((L18-L22) AND L15) OR (L15 AND L16)

=> d que l23
L5                STR
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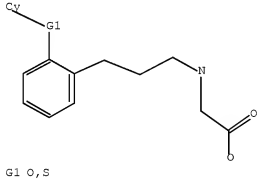


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 G1 O,S


Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str
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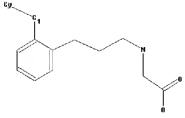
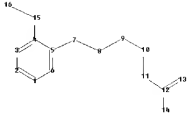


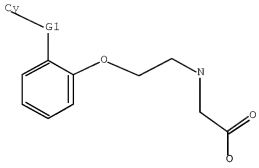


chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
5-7 7-8 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

L9 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation:

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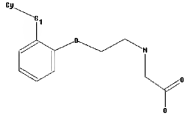
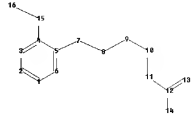


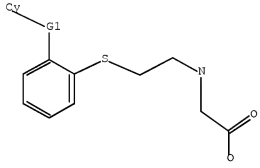


chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

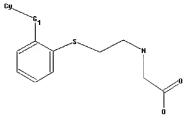
L11 STR

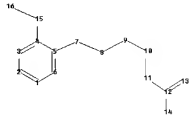


G1 O,S

Structure attributes must be viewed using STN Express query preparation:

Uploading L6.str





chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :

```
8-9  9-10  10-11
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
4-15  5-7  7-8  8-9  9-10  10-11  12-13  12-14  15-16
exact bonds :
11-12
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 :


G1:O,S

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:Atom
Generic attributes :
16:
Type of Ring System    : Monocyclic




L14         171 SEA FILE=REGISTRY SSS FUL L5 OR L9 OR L11
L15          11 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L14
L16           1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  US20060235003/PN
L18           6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SMITH GARRICK/AU
L19          17 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MIKKELSEN G?/AU
L20          71 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ANDERSEN KIM/AU
L21         203 SEA FILE=HCAPLUS ABB=ON  PLU=ON  GREVE D?/AU
L22          19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ESKILDSEN J?/AU
L23           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (((L18 OR L19 OR L20 OR L21
                OR L22)) AND L15) OR (L15 AND L16)


=> d l23 1-2 ibib abs hitstr

L23  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2006:625349  HCAPLUS  Full-text
DOCUMENT NUMBER:          145:224321
TITLE:                    The synthesis and SAR of
                          2-arylsulfanylphenyl-1-oxyalkylamino acids as GlyT-1
                          inhibitors
AUTHOR(S):                Smith, Garrick; Mikkelsen, Gitte;
                          Eskildsen, Jorgen; Bundgaard, Christoffer
CORPORATE SOURCE:         Medicinal Chemistry Research, H. Lundbeck A/S, Valby,
                          DK 2500, Den.
SOURCE:                   Bioorganic & Medicinal Chemistry Letters (2006),
                          16(15), 3981-3984
                          CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER:                Elsevier B.V.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 145:224321
GI
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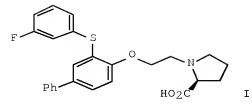


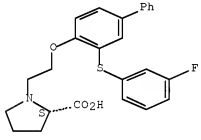
I

AB Elevation of glycine levels by inhibition of the glycine transporter-1 (GlyT-1) and activation of the NMDA receptor is a potential strategy for the treatment of schizophrenia. A novel series of 2-arylsulfanylphenyl-1-oxyalkyl amino acids have been identified. The most prominent member of this series (I) is a potent GlyT-1 inhibitor (IC50 = 59 nM). In vitro and in vivo assessment of CNS exposure indicates this compound is a likely substrate for active efflux transporters.

IT 791644-20-7P 791644-21-8P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and SAR of arylsulfanylphenyloxyalkylamino acids as GlyT-1 inhibitors)

RN 791644-20-7 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 791644-21-8 HCAPLUS
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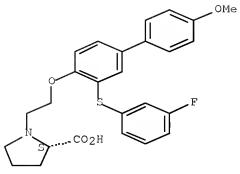
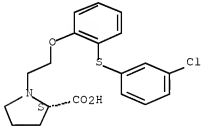
Absolute stereochemistry.



IT 791642-87-0P 791643-06-6P 791643-10-2P
791643-25-9P 791643-27-1P 791643-31-7P
791643-68-0P 791644-17-2P 791644-18-3P
794510-03-5P 905815-53-4P 905815-54-5P
905815-55-6P 905815-56-7P 905815-57-8P
905815-58-9P 905815-59-0P 905815-60-3P
905815-61-4P 905815-62-5P 905815-63-6P
905815-64-7P 905815-65-8P 905815-66-9P
905815-67-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and SAR of arylsulfanylphenyloxyalkylamino acids as GlyT-1 inhibitors)
RN 791642-87-0 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



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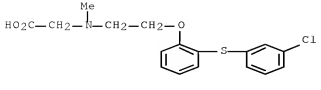

RN 791643-10-2 HCAPLUS
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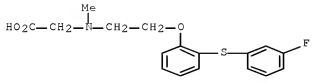

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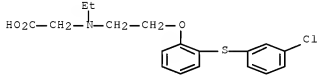

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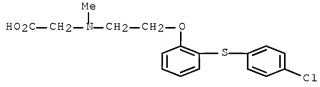

RN 791643-31-7 HCAPLUS
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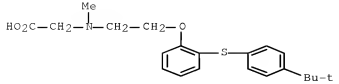
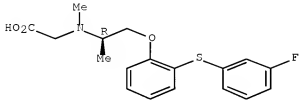


RN 791643-68-0 HCAPLUS
CN Glycine, N-[(1R)-2-[2-[(3-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 791644-17-2 HCAPLUS
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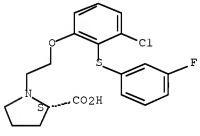
Absolute stereochemistry.



RN 791644-18-3 HCAPLUS
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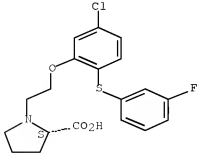
Absolute stereochemistry.



RN 794510-03-5 HCAPLUS
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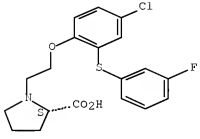
Absolute stereochemistry.



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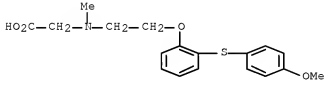

RN 905815-54-5 HCAPLUS
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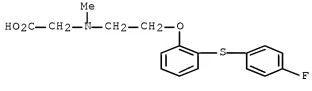

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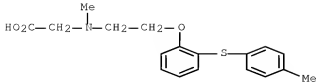

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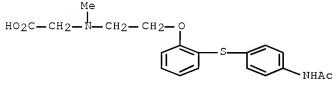
(CA INDEX NAME)



RN 905815-57-8 HCAPLUS
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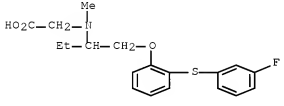
(CA INDEX NAME)



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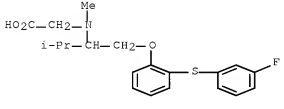
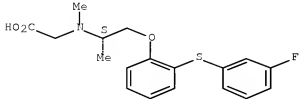
methyl- (CA INDEX NAME)



RN 905815-59-0 HCAPLUS

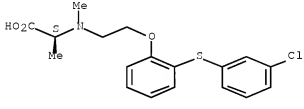
CN Glycine, N-[(1S)-2-[2-[(3-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



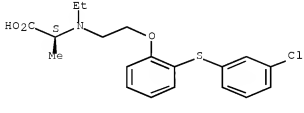
RN 905815-60-3 HCAPLUS
CN L-Alanine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



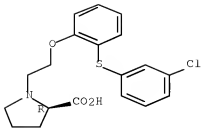
RN 905815-61-4 HCAPLUS
CN L-Alanine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)

Absolute stereochemistry.



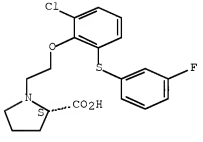
RN 905815-62-5 HCAPLUS
CN D-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



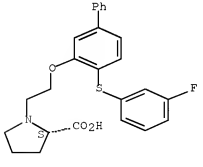
RN 905815-63-6 HCAPLUS
CN L-Proline, 1-[2-[2-chloro-6-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



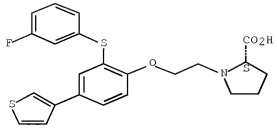
RN 905815-64-7 HCAPLUS
CN L-Proline, 1-[2-[[4-[(3-fluorophenyl)thio][1,1'-biphenyl]-3-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



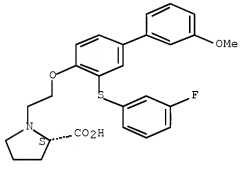
RN 905815-65-8 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(3-thienyl)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



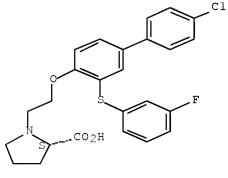
RN 905815-66-9 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-3'-methoxy[1,1'-biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 905815-67-0 HCAPLUS
CN L-Proline, 1-[2-[[4'-chloro-3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

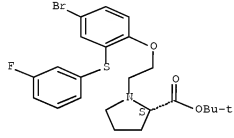


IT 791642-79-0P 791644-01-4P 905816-02-6P
905816-03-7P 905816-06-0P 905816-07-1P
905816-08-2P 905816-09-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and SAR of arylsulfanylphenyloxyalkylamino acids as GlyT-1 inhibitors)

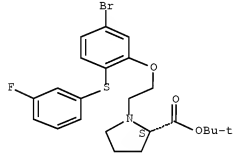
RN 791642-79-0 HCAPLUS
CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



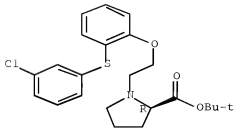
RN 791644-01-4 HCAPLUS
CN L-Proline, 1-[2-[5-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



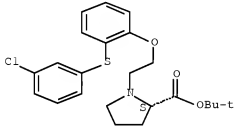
RN 905816-02-6 HCAPLUS
CN D-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



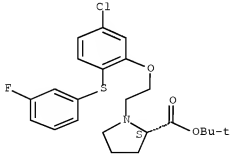
RN 905816-03-7 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



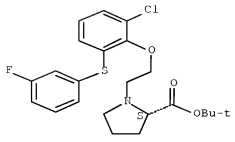
RN 905816-06-0 HCAPLUS
CN L-Proline, 1-[2-[5-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



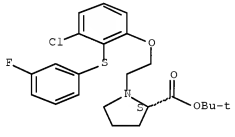
RN 905816-07-1 HCAPLUS
CN L-Proline, 1-[2-[2-chloro-6-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



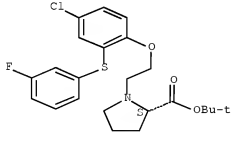
RN 905816-08-2 HCAPLUS
CN L-Proline, 1-[2-[3-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 905816-09-3 HCAPLUS
CN L-Proline, 1-[2-[4-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:965214 HCAPLUS Full-text
DOCUMENT NUMBER: 141:411217
TITLE: A preparation of oxyphenyl and sulfanylphenyl

derivatives of amino acids, useful as glycine transporter inhibitors

INVENTOR(S): Smith, Garrick Paul; Mikkelsen, Gitte; Andersen, Kim; Greve, Daniel Rodriguez ; Eskildsen, Joergen

PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.

SOURCE: PCT Int. Appl., 87 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004096761	A1	20041111	WO 2004-DK290	20040427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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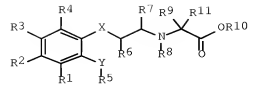
CA 2523585	A1	20041111	CA 2004-2523585	20040427
EP 1622868	A1	20060208	EP 2004-729612	20040427
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004009739	A	20060509	BR 2004-9739	20040427
CN 1780815	A	20060531	CN 2004-80011219	20040427
JP 2006524642	T	20061102	JP 2006-504368	20040427
MX 2005011198	A	20051214	MX 2005-11198	20051018
IN 2005CN02812	A	20070525	IN 2005-CN2812	20051031
NO 2005005632	A	20051129	NO 2005-5632	20051129
US 20060235003	A1	20061019	US 2006-551737	20060606 <--

PRIORITY APPLN. INFO.:			
	DK 2003-649	A	20030430
	US 2003-466755P	P	20030430
	WO 2004-DK290	W	20040427

OTHER SOURCE(S): MARPAT 141:411217

GI



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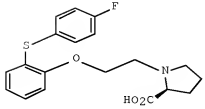

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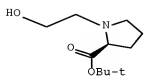


III

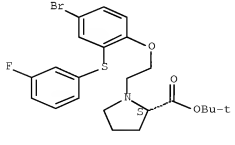
AB The invention relates to a preparation of aromatic oxyphenyl and aromatic sulfanylphenyl derivs. of formula I [wherein: X is O, S, or CH2, etc.; Y is O or S; R1, R2, R3, and R4 are independently selected from H, halogen, CN, NO2, or alk(en/yn)yl, etc.; R5 is (un)substituted aryl or monocyclic heteroaryl; R6 is H, alk(en/yn)yl, cycloalk(en)yl, or alk(en/yn)ylsulfanyl, etc.; R7 and R8 are independently selected from H, alk(en/yn)yl, or cycloalk(en)yl; R9 and R11 are independently selected from H, alk(en/yn)yl, hydroxyalk(en/yn)yl, or alk(en/yn)ylsulfanyl, etc.; R10 is H, alk(en/yn)yl, aryl, or arylalk(en/yn)yl, etc.; R6 and R8 together with the nitrogen may form 3-7 membered heterocyclic ring], useful as glycine transporter inhibitors (IC50 < 10000 nM). The compds. of formula I are useful for the treatment of diseases such as schizophrenia, including both the pos. and the neg. symptoms of schizophrenia. For instance, pyrrolidinecarboxylic acid derivative II was prepared via etherification of 2-(3-fluorophenylsulfanyl)phenol by (hydroxyethyl)pyrrolidinecarboxylate derivative III.

IT 791642-79-0P, (S)-1-[2-[4-Bromo-2-(3-fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of oxyphenyl and sulfanylphenyl derivs. of amino acids, useful as glycine transporter inhibitors)

RN 791642-79-0 HCAPLUS

CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

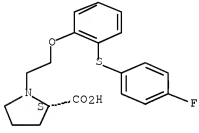


IT 791642-81-4P, (S)-1-[2-[2-(4-Fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-83-6P, (S)-1-[2-[2-(4-tert-Butylphenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-84-7P, (S)-1-[2-[2-(4-Trifluoromethylphenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-85-8P, (S)-1-[2-[2-(3-Fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-86-9P, (S)-1-[2-[2-(4-Chlorophenylsulfanyl)-phenoxy]-ethyl]pyrrolidine-2-carboxylic acid 791642-87-0P, (S)-1-[2-[2-(3-Chlorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-88-1P, (S)-1-[2-[2-(3,4-Dichlorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-90-5P, (S)-1-[2-[2-(3-Chloro-4-fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-91-6P, (S)-1-[2-[2-(3-Chlorophenoxy)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-92-7P 791642-93-8P 791642-94-9P 791642-95-0P 791642-97-2P 791642-98-3P 791642-99-4P 791643-00-0P 791643-01-1P 791643-02-2P 791643-04-4P 791643-06-6P 791643-08-8P 791643-10-2P 791643-12-4P 791643-14-6P 791643-16-8P 791643-17-9P 791643-18-0P 791643-20-4P 791643-21-5P 791643-22-6P, 3-[2-(4-tert-Butylphenylsulfanyl)phenoxy]pyrrolidin-1-ylacetic acid 791643-25-9P 791643-27-1P, [[2-[2-(4-Chlorophenylsulfanyl)phenoxy]ethyl]-N-methylamino]acetic acid 791643-29-3P, 2-[3-[2-(4-Trifluoromethylphenylsulfanyl)phenoxy]pyrrolidin-1-yl]propionic acid 791643-30-6P, [[2-[2-(4-tert-Butylphenylsulfanyl)phenoxy]ethyl]-N-isopropylamino]acetic acid 791643-31-7P, [[2-[2-(4-tert-Butylphenylsulfanyl)phenoxy]ethyl]-N-methylamino]acetic acid 791643-33-9P, [[2-[2-(3,4-Dichlorophenylsulfanyl)phenoxy]ethyl]-N-methylamino]acetic acid 791643-34-0P 791643-35-1P 791643-37-3P 791643-38-4P 791643-39-5P 791643-41-9P 791643-42-0P 791643-45-3P, [[1-[2-(3,4-Dichlorophenylsulfanyl)phenoxy]butan-2-yl]-N-ethylamino]acetic acid 791643-46-4P 791643-48-6P 791643-49-7P 791643-51-1P 791643-52-2P 791643-53-3P 791643-55-5P 791643-57-7P 791643-58-8P 791643-63-5P 791643-65-7P 791643-66-8P 791643-68-0P 791643-70-4P 791643-71-5P 791643-72-6P 791643-73-7P 791643-74-8P 791643-75-9P 791643-76-0P 791643-77-1P 791643-78-2P 791643-79-3P 791643-80-6P 791643-81-7P 791643-84-0P 791643-85-1P 791643-86-2P 791643-87-3P 791643-88-4P 791643-90-8P 791643-91-9P 791643-92-0P 791643-94-2P 791643-95-3P 791643-97-5P 791643-99-7P 791644-00-3P 791644-02-5P 791644-04-7P 791644-06-9P 791644-08-1P 791644-09-2P 791644-10-5P 791644-11-6P 791644-12-7P 791644-15-0P 791644-16-1P 791644-17-2P 791644-18-3P 791644-19-4P 791644-20-7P 791644-21-8P 791644-22-9P 791644-23-0P 791644-24-1P 791644-25-2P 791644-26-3P 791644-27-4P 791644-28-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxyphenyl and sulfanylphenyl derivs. of amino acids, useful as glycine transporter inhibitors)

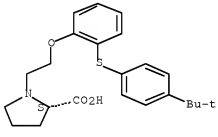
RN 791642-81-4 HCAPLUS
CN L-Proline, 1-[2-[2-[(4-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



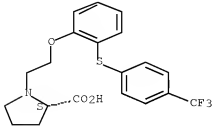
RN 791642-83-6 HCAPLUS
CN L-Proline, 1-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



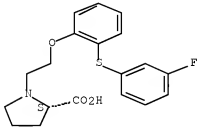
RN 791642-84-7 HCAPLUS
CN L-Proline, 1-[2-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



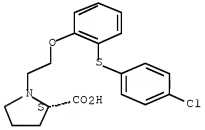
RN 791642-85-8 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



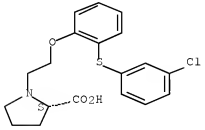
RN 791642-86-9 HCAPLUS
CN L-Proline, 1-[2-[2-[(4-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 791642-87-0 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

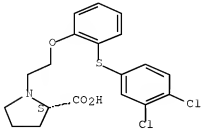
Absolute stereochemistry.



RN 791642-88-1 HCAPLUS
CN L-Proline, 1-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]ethyl]- (CA INDEX

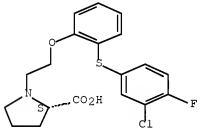
NAME)

Absolute stereochemistry.



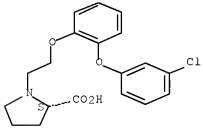
RN 791642-90-5 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



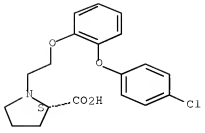
RN 791642-91-6 HCAPLUS
CN L-Proline, 1-[2-[2-(3-chlorophenoxy)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



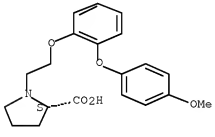
RN 791642-92-7 HCAPLUS
CN L-Proline, 1-[2-[2-(4-chlorophenoxy)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



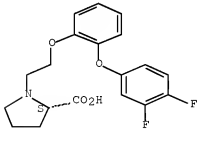
RN 791642-93-8 HCAPLUS
CN L-Proline, 1-[2-[2-(4-methoxyphenoxy)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



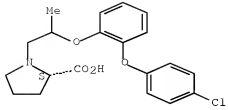
RN 791642-94-9 HCAPLUS
CN L-Proline, 1-[2-[2-(3,4-difluorophenoxy)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



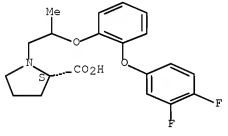
RN 791642-95-0 HCAPLUS
CN L-Proline, 1-[2-[2-(4-chlorophenoxy)phenoxy]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



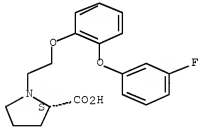
RN 791642-97-2 HCAPLUS
CN L-Proline, 1-[2-[2-(3,4-difluorophenoxy)phenoxy]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



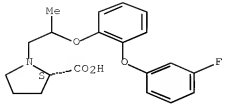
RN 791642-98-3 HCAPLUS
CN L-Proline, 1-[2-[2-(3-fluorophenoxy)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



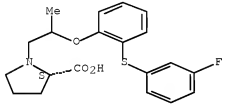
RN 791642-99-4 HCAPLUS
CN L-Proline, 1-[2-[2-(3-fluorophenoxy)phenoxy]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



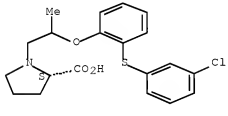
RN 791643-00-0 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]phenoxy]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

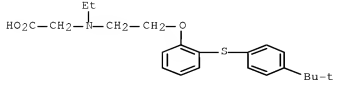


RN 791643-01-1 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]propyl]- (CA INDEX NAME)

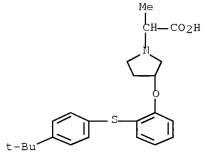
Absolute stereochemistry.



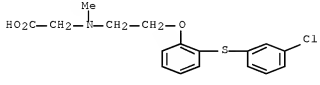
RN 791643-02-2 HCAPLUS
CN Glycine, N-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-N-ethyl-
(CA INDEX NAME)



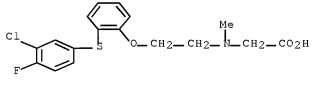
RN 791643-04-4 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-α-methyl- (CA INDEX NAME)



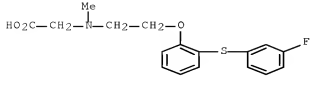
RN 791643-06-6 HCAPLUS
CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



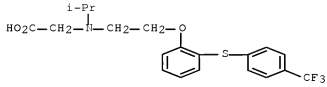
RN 791643-08-8 HCAPLUS
CN Glycine, N-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



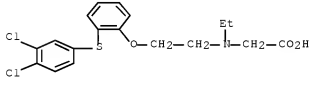
RN 791643-10-2 HCAPLUS
CN Glycine, N-[2-[2-[(3-fluorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



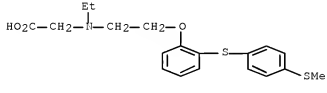
RN 791643-12-4 HCAPLUS
CN Glycine, N-(1-methylethyl)-N-[2-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)



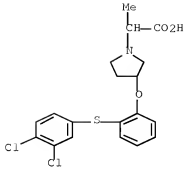
RN 791643-14-6 HCAPLUS
CN Glycine, N-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)



RN 791643-16-8 HCAPLUS
CN Glycine, N-ethyl-N-[2-[2-[[4-(methylthio)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)

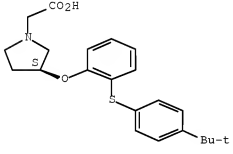


RN 791643-17-9 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[(3,4-dichlorophenyl)thio]phenoxy]-α-methyl- (CA INDEX NAME)

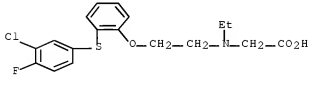


RN 791643-18-0 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-, (3S)- (CA INDEX NAME)

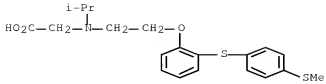
Absolute stereochemistry.



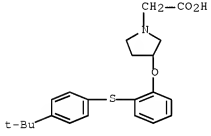
RN 791643-20-4 HCAPLUS
CN Glycine, N-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)



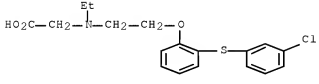
RN 791643-21-5 HCAPLUS
CN Glycine, N-(1-methylethyl)-N-[2-[2-[[4-(methylthio)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)



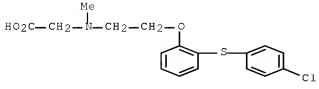
RN 791643-22-6 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]- (CA INDEX NAME)



RN 791643-25-9 HCAPLUS
CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)

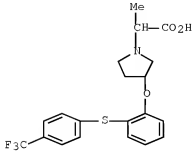


RN 791643-27-1 HCAPLUS
CN Glycine, N-[2-[2-[(4-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)

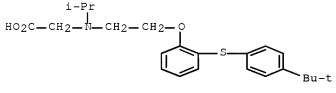


RN 791643-29-3 HCAPLUS

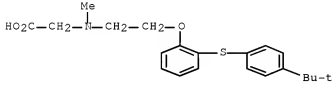
CN 1-Pyrrolidineacetic acid, α-methyl-3-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]- (CA INDEX NAME)



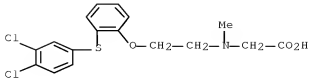
RN 791643-30-6 HCAPLUS
CN Glycine, N-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-N-(1-methylethyl)- (CA INDEX NAME)



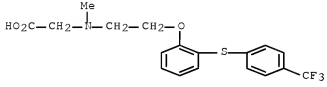
RN 791643-31-7 HCAPLUS
CN Glycine, N-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 791643-33-9 HCAPLUS
CN Glycine, N-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)

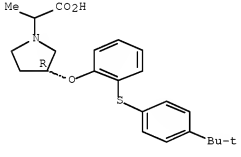


RN 791643-34-0 HCAPLUS
CN Glycine, N-methyl-N-[2-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]ethyl]-
(CA INDEX NAME)



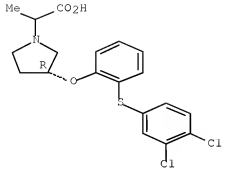
RN 791643-35-1 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-
α-methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



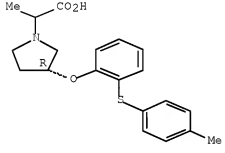
RN 791643-37-3 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[(3,4-dichlorophenyl)thio]phenoxy]-α-
methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



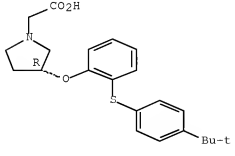
RN 791643-38-4 HCAPLUS
CN 1-Pyrrolidineacetic acid, α-methyl-3-[2-[(4-methylphenyl)thio]phenoxy]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



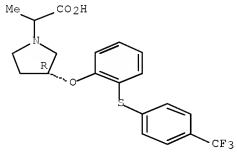
RN 791643-39-5 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



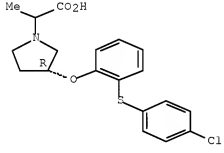
RN 791643-41-9 HCAPLUS
CN 1-Pyrrolidineacetic acid, α-methyl-3-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

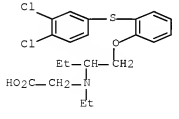


RN 791643-42-0 HCAPLUS
CN 1-Pyrrolidineacetic acid, 3-[2-[(4-chlorophenyl)thio]phenoxy]-α-methyl-, (3R)- (CA INDEX NAME)

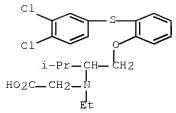
Absolute stereochemistry.



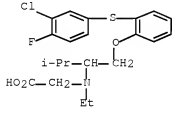
RN 791643-45-3 HCAPLUS
CN Glycine, N-[1-[[2-[(3,4-dichlorophenyl)thio]phenoxy]methyl]propyl]-N-ethyl- (CA INDEX NAME)



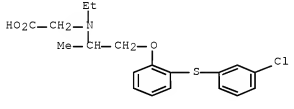
RN 791643-46-4 HCAPLUS
CN Glycine, N-[1-[[2-[(3,4-dichlorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-ethyl- (CA INDEX NAME)



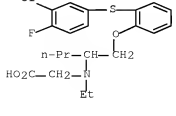
RN 791643-48-6 HCAPLUS
CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-ethyl- (CA INDEX NAME)



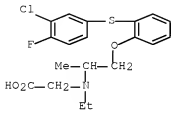
RN 791643-49-7 HCAPLUS
CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)



RN 791643-51-1 HCAPLUS
CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]butyl]-N-ethyl- (CA INDEX NAME)

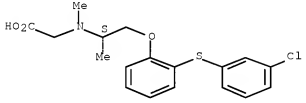


RN 791643-52-2 HCAPLUS
CN Glycine, N-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)



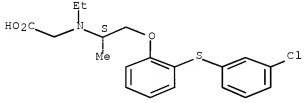
RN 791643-53-3 HCAPLUS
CN Glycine, N-[(1S)-2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

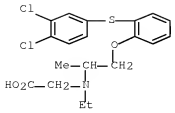


RN 791643-55-5 HCAPLUS
CN Glycine, N-[(1S)-2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)

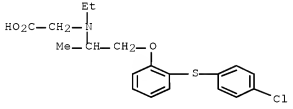
Absolute stereochemistry.



RN 791643-57-7 HCAPLUS
CN Glycine, N-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)

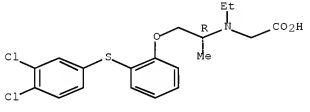


RN 791643-58-8 HCAPLUS
CN Glycine, N-[2-[2-[(4-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl-
(CA INDEX NAME)



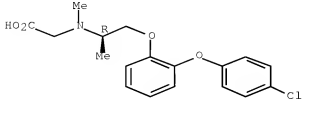
RN 791643-63-5 HCAPLUS
CN Glycine, N-[(1R)-2-[2-[(3,4-dichlorophenyl)thio]phenoxy]-1-methylethyl]-N-
ethyl- (CA INDEX NAME)

Absolute stereochemistry.



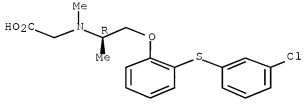
RN 791643-65-7 HCAPLUS
CN Glycine, N-[(1R)-2-[2-(4-chlorophenoxy)phenoxy]-1-methylethyl]-N-methyl-
(CA INDEX NAME)

Absolute stereochemistry.



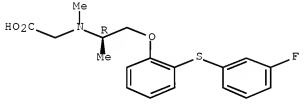
RN 791643-66-8 HCAPLUS
CN Glycine, N-[(1R)-2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

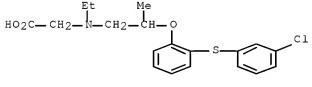


RN 791643-68-0 HCAPLUS
CN Glycine, N-[(1R)-2-[2-[(3-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

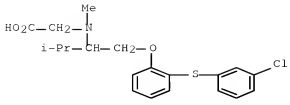
Absolute stereochemistry.



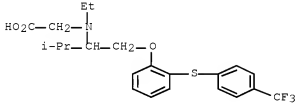
RN 791643-70-4 HCAPLUS
CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]propyl]-N-ethyl- (CA INDEX NAME)



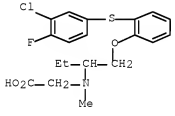
RN 791643-71-5 HCAPLUS
CN Glycine, N-[1-[[2-[(3-chlorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-methyl- (CA INDEX NAME)



RN 791643-72-6 HCAPLUS
CN Glycine, N-ethyl-N-[2-methyl-1-[[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]methyl]propyl]- (CA INDEX NAME)

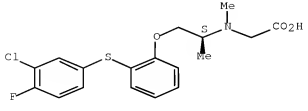


RN 791643-73-7 HCAPLUS
CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]propyl]-N-methyl- (CA INDEX NAME)



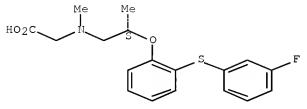
RN 791643-74-8 HCAPLUS
CN Glycine, N-[(1S)-2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

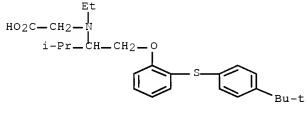


RN 791643-75-9 HCAPLUS
CN Glycine, N-[(2S)-2-[2-[(3-fluorophenyl)thio]phenoxy]propyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

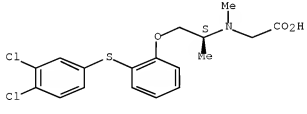


RN 791643-76-0 HCAPLUS
CN Glycine, N-[1-[[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]methyl]-2-methylpropyl]-N-ethyl- (CA INDEX NAME)

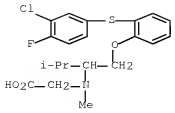


RN 791643-77-1 HCAPLUS
CN Glycine, N-[(1S)-2-[2-[(3,4-dichlorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

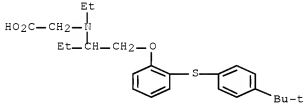
Absolute stereochemistry.



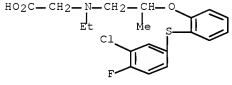
RN 791643-78-2 HCAPLUS
CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-methyl- (CA INDEX NAME)



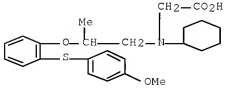
RN 791643-79-3 HCAPLUS
CN Glycine, N-[1-[[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]methyl]propyl]-N-ethyl- (CA INDEX NAME)



RN 791643-80-6 HCAPLUS
CN Glycine, N-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]propyl]-N-ethyl- (CA INDEX NAME)

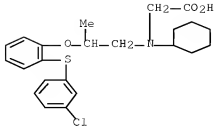


RN 791643-81-7 HCAPLUS
CN Glycine, N-cyclohexyl-N-[2-[2-[(4-methoxyphenyl)thio]phenoxy]propyl]- (CA INDEX NAME)



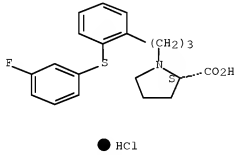
RN 791643-84-0 HCAPLUS
CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]propyl]-N-cyclohexyl- (CA

INDEX NAME)



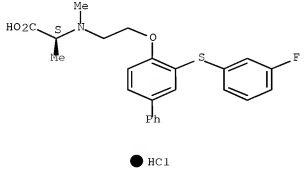
RN 791643-85-1 HCAPLUS
CN L-Proline, 1-[3-[2-[(3-fluorophenyl)thio]phenyl]propyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



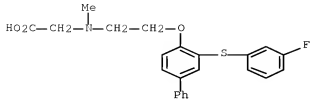
RN 791643-86-2 HCAPLUS
CN L-Alanine, N-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



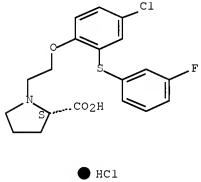
RN 791643-87-3 HCAPLUS

CN Glycine, N-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-N-methyl- (CA INDEX NAME)



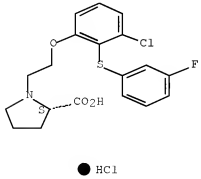
RN 791643-88-4 HCAPLUS
CN L-Proline, 1-[2-[4-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



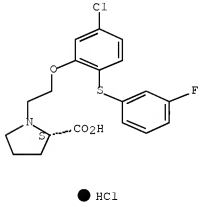
RN 791643-90-8 HCAPLUS
CN L-Proline, 1-[2-[3-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



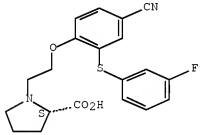
RN 791643-91-9 HCAPLUS
CN L-Proline, 1-[2-[5-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



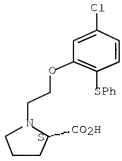
RN 791643-92-0 HCAPLUS
CN L-Proline, 1-[2-[4-cyano-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



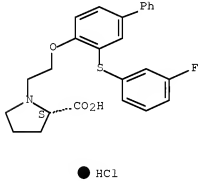
RN 791643-94-2 HCAPLUS
CN L-Proline, 1-[2-[5-chloro-2-(phenylthio)phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



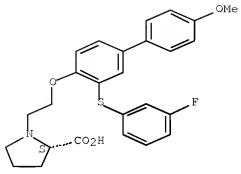
RN 791643-95-3 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 791643-97-5 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-4'-methoxy[1,1'-biphenyl]-4-yl]oxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

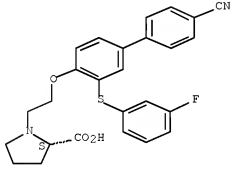
Absolute stereochemistry.



● HCl

RN 791643-99-7 HCAPLUS
CN L-Proline, 1-[2-[[4'-cyano-3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

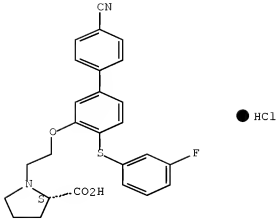
Absolute stereochemistry.



● HCl

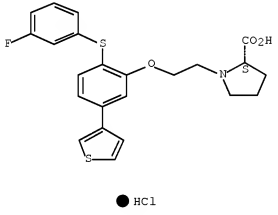
RN 791644-00-3 HCAPLUS
CN L-Proline, 1-[2-[[4'-cyano-4-[(3-fluorophenyl)thio][1,1'-biphenyl]-3-yl]oxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



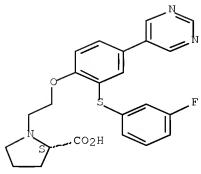
RN 791644-02-5 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-5-(3-thienyl)phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 791644-04-7 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(5-pyrimidinyl)phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

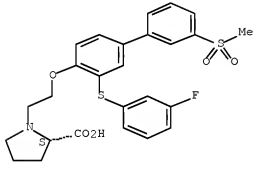
Absolute stereochemistry.



● HCl

RN 791644-06-9 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-3'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]oxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

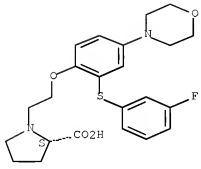
Absolute stereochemistry.



● HCl

RN 791644-08-1 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(4-morpholinyl)phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

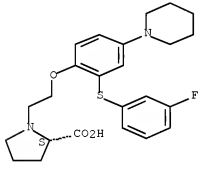
Absolute stereochemistry.



● HCl

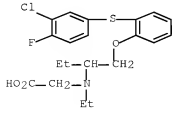
RN 791644-09-2 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(1-piperidinyl)phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



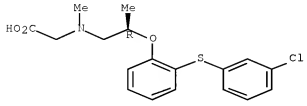
● HCl

RN 791644-10-5 HCAPLUS
CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]propyl]-N-ethyl- (CA INDEX NAME)

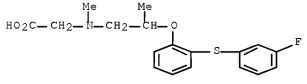


RN 791644-11-6 HCAPLUS
CN Glycine, N-[(2R)-2-[2-[(3-chlorophenyl)thio]phenoxy]propyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

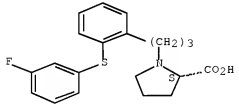


RN 791644-12-7 HCAPLUS
CN Glycine, N-[2-[2-[(3-fluorophenyl)thio]phenoxy]propyl]-N-methyl- (CA INDEX NAME)



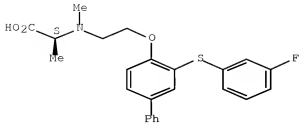
RN 791644-15-0 HCAPLUS
CN L-Proline, 1-[3-[2-[(3-fluorophenyl)thio]phenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



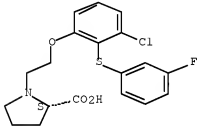
RN 791644-16-1 HCAPLUS
CN L-Alanine, N-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



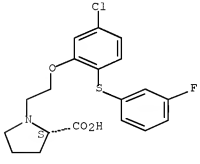
RN 791644-17-2 HCAPLUS
CN L-Proline, 1-[2-[3-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



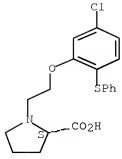
RN 791644-18-3 HCAPLUS
CN L-Proline, 1-[2-[5-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



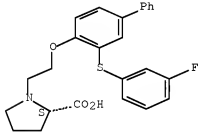
RN 791644-19-4 HCAPLUS
CN L-Proline, 1-[2-[5-chloro-2-(phenylthio)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



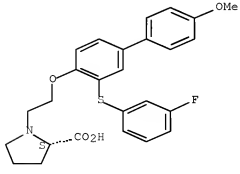
RN 791644-20-7 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-
(CA INDEX NAME)

Absolute stereochemistry.



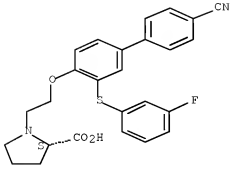
RN 791644-21-8 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-4'-methoxy[1,1'-biphenyl]-4-
yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



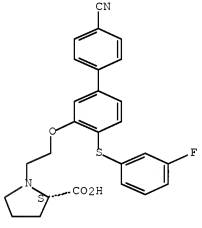
RN 791644-22-9 HCAPLUS
CN L-Proline, 1-[2-[[4'-cyano-3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-
yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



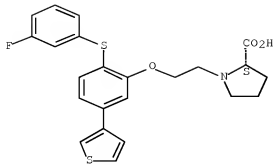
RN 791644-23-0 HCAPLUS
CN L-Proline, 1-[2-[[4'-cyano-4-[(3-fluorophenyl)thio][1,1'-biphenyl]-3-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



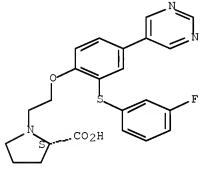
RN 791644-24-1 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-5-(3-thienyl)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



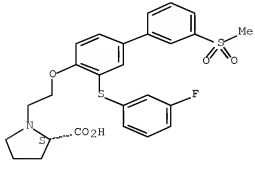
RN 791644-25-2 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(5-pyrimidinyl)phenoxy]ethyl]-
(CA INDEX NAME)

Absolute stereochemistry.



RN 791644-26-3 HCAPLUS
CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-3'-(methylsulfonyl)[1,1'-
biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

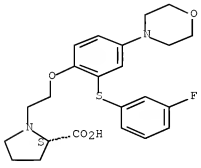
Absolute stereochemistry.



RN 791644-27-4 HCAPLUS

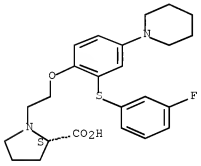
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(4-morpholinyl)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



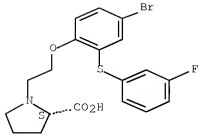
RN 791644-28-5 HCAPLUS
CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(1-piperidinyl)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



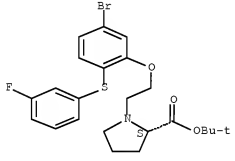
IT 791643-98-6 791644-01-4 791644-07-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of oxyphenyl and sulfanylphenyl derivs. of amino acids, useful as glycine transporter inhibitors)
RN 791643-98-6 HCAPLUS
CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



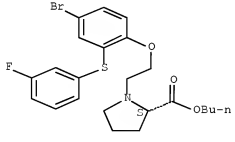
RN 791644-01-4 HCAPLUS
CN L-Proline, 1-[2-[5-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 791644-07-0 HCAPLUS
CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, butyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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     (FILE 'HCAPLUS' ENTERED AT 13:11:11 ON 26 MAR 2009)
L24            9 S L15 NOT L23

=> d que l24
L5                STR
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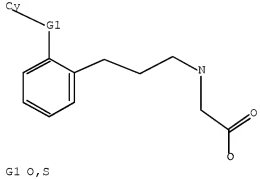
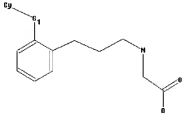
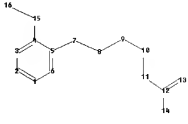


G1 O,S

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



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7  12  13  14  15  16
ring nodes :
1  2  3  4  5  6
ring/chain nodes :
8  9  10  11
chain bonds :
4-15  5-7  7-8  11-12  12-13  12-14  15-16
ring/chain bonds :
8-9  9-10  10-11
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
4-15  8-9  9-10  10-11  12-13  12-14  15-16
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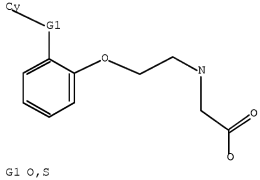
exact bonds :
5-7 7-8 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

L9 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation:

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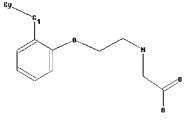
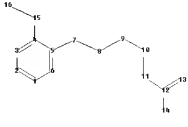


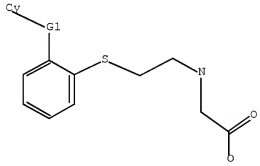


chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

L11 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation:

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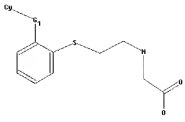

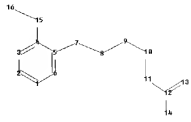

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chain nodes :
7  12  13  14  15  16
ring nodes :
1  2  3  4  5  6
ring/chain nodes :
8  9  10  11
chain bonds :
4-15  5-7  7-8  11-12  12-13  12-14  15-16
ring/chain bonds :
8-9  9-10  10-11
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
4-15  5-7  7-8  8-9  9-10  10-11  12-13  12-14  15-16
exact bonds :
11-12
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 :


G1:O,S

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:Atom
Generic attributes :
16:
Type of Ring System    : Monocyclic
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L16            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  US20060235003/PN
L18            6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SMITH GARRICK/AU
L19           17 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MIKKELSEN G?/AU
L20           71 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ANDERSEN KIM/AU
L21          203 SEA FILE=HCAPLUS ABB=ON  PLU=ON  GREVE D?/AU
L22           19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ESKILDSEN J?/AU
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                OR L22)) AND L15) OR (L15 AND L16)
L24           9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15 NOT L23


=> d l24 1-9 ibib abs hitstr

L24  ANSWER 1 OF 9  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2006:1093266  HCAPLUS  Full-text
DOCUMENT NUMBER:          145:432223
TITLE:                    Method of treating schizophrenia prodrome
INVENTOR(S):              Woods, Scott W.
PATENT ASSIGNEE(S):       Yale University, USA
SOURCE:                   PCT Int. Appl., 64pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.            KIND   DATE        APPLICATION NO.          DATE
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     WO 2006110724          A2    20061019    WO 2006-US13444          20060411
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
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     EP 1871165             A2    20080102    EP 2006-740849           20060411
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             BA, HR, MK, YU
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PRIORITY APPLN. INFO.:                       US 2005-670600P      P   20050411
                                             WO 2006-US13444      W   20060411
OTHER SOURCE(S):          MARPAT 145:432223
AB   The present invention relates to a method of treating schizophrenia prodrome
     in human subjects using a NMDA glycine site agonist, a glycine transporter-1
     inhibitor or mixts. thereof, optionally in combination with a pharmaceutically
     acceptable additive, carrier or excipient.
IT   791642-83-6
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (method of treating schizophrenia prodrome with NMDA glycine agonist
        and glycine transporter-1 inhibitor)
RN   791642-83-6  HCAPLUS
CN   L-Proline, 1-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-  (CA
     INDEX NAME)

Absolute stereochemistry.
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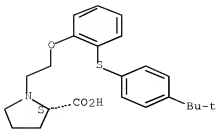


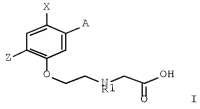
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1154515 HCAPLUS Full-text
DOCUMENT NUMBER: 143:422634
TITLE: Preparation of N-(2-aryloxyethyl)glycine derivatives and their use as glycine transport inhibitors
INVENTOR(S): Man, Teresa; Milot, Guy; Porter, Warren Jaye; Reel, Jon Kevin; Rudyk, Helene Catherine Eugenie; Valli, Matthew John; Walter, Magnus Wilhelm
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 187 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005100301	A1	20051027	WO 2005-US8962	20050318

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-558260P P 20040331
OTHER SOURCE(S): CASREACT 143:422634; MARPAT 143:422634
GI



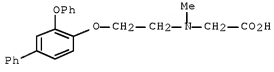
I

AB The invention relates to (aryloxyethyl)glycine derivs. I [X is H, halo, alkyl, CF3, cycloalkyl, arylcarbonyl, (un)substituted aryl, fused aryicycloalkyl or heteroaryl, fused arylheterocyclyl; Z is alkyl, alkenyl, Y, CO-Y, CH(OH)-Y, OY, alkyl-Y, alkyl-OY, SY, CF2Y or NR2-Y, where Y is alkyl, (CH2)1-10CF3, CF3, C2F5, C3F7, (un)substituted aryl, heteroaryl, cycloalkyl or heterocyclyl and R2 is H or alkyl; A is (un)substituted aryl, H, alkoxy; R1 is alkyl] or their pharmaceutically-acceptable salts that exhibit activity as inhibitors of the glycine type-1 transporter, to pharmaceutical compns. containing them and to their use in the treatment of neurol. and neuropsychiatric disorders. Thus, glycine derivative I (X = Ph, Z = 2-thienyl, A = H, R1 = H) was prepared via reactions of 3-iodo-4-methoxybiphenyl, 2-thiopheneboronic acid, and [(2-hydroxyethyl)methylamino]acetic acid tert-Bu ester.

IT 868263-52-9P 868264-97-5P 868265-44-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (aryloxyethyl)glycine derivs. as glycine transport inhibitors)

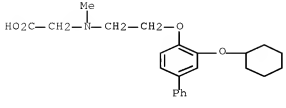
RN 868263-52-9 HCAPLUS

CN Glycine, N-methyl-N-[2-[(3-phenoxy[1,1'-biphenyl]-4-yl)oxy]ethyl]- (CA INDEX NAME)

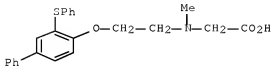


RN 868264-97-5 HCAPLUS

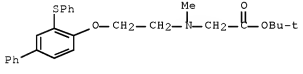
CN Glycine, N-[2-[[3-(cyclohexyloxy)[1,1'-biphenyl]-4-yl]oxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 868265-44-5 HCAPLUS
CN Glycine, N-methyl-N-[2-[[3-(phenylthio)[1,1'-biphenyl]-4-yl]oxy]ethyl]-
(CA INDEX NAME)



IT 868263-20-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (aryloxyethyl)glycine derivs. as glycine transport inhibitors)
RN 868263-20-1 HCAPLUS
CN Glycine, N-methyl-N-[2-[[3-(phenylthio)[1,1'-biphenyl]-4-yl]oxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



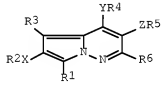
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:878155 HCAPLUS Full-text
DOCUMENT NUMBER: 141:366240
TITLE: Preparation of pyrrolopyridazines for the treatment of proliferative disorders
INVENTOR(S): Salvati, Mark E.; Illig, Carl R.; Wilson, Kenneth Jerome; Chen, Jinsheng; Meegalla, Sanath K.; Wall, Mark James
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: U.S. Pat. Appl. Publ., 189 pp., Cont.-in-part of U.S. Ser. No. 396,197.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040209886	A1	20041021	US 2003-672850	20030926
US 7030112	B2	20060418		
US 20040063712	A1	20040401	US 2003-396197	20030325

US 6900208 B2 20050531
WO 2005030144 A2 20050407 WO 2004-US31571 20040923
WO 2005030144 A3 20051027
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1664051 A2 20060607 EP 2004-789070 20040923
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
US 20050159420 A1 20050721 US 2005-29547 20050105
PRIORITY APPLN. INFO.: US 2003-396197 A2 20030325
US 2002-368249P P 20020328
US 2002-402118P P 20020808
US 2003-672850 A 20030926
WO 2004-US31571 W 20040923

OTHER SOURCE(S): MARPAT 141:366240
GI



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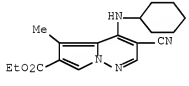


II

AB Pyrrolopyridazines I [R1 = H, alkyl, aralkyl, halo, OH, etc.; R2 = alkyl, cycloalkyl, aryl, heterocyclic, aralkyl, (un)substituted CO2H, CHO, CONH2, SO3H, SO2NH2, SH, S(O)H, SO2H; R1R2, R2R3 = cycloalkyl, aryl, heterocyclic; R3 = H, alkyl, cycloalkyl, heterocyclic, aryl, aralkyl, acyl, halo, (un)substituted OH, CH2OH, CH2NH2, CH2SH; R4 = alkyl, cycloalkyl, aryl, heterocyclic, aralkyl, acyl, (un)substituted CO2H, CONH2, SO3H, SO2NH2, SH, S(O)H, SO2H; R5 = H, halo, CN, alkyl, cycloalkyl, heterocyclic, aryl, aralkyl, acyl, alkylene, (un)substituted CO2H, CONH2, SO3H, SO2NH2, SH, S(O)H, SO2H; R6 = H, alkyl, cycloalkyl, aryl, aralkyl, heterocyclic, acyl, alkoxycarbonyl, carbamoyl; X, Y, Z = bond, O, S, (un)substituted NH, etc.] were prepared for use in the treatment of proliferative, inflammatory, and other disorders (no data). Thus, NCCH2CO2Et was cyclized with MeCHO to di-Et 3-methyl-1H-pyrrole-2,4-dicarboxylate which was N-aminated and cyclized with (EtO)2CHCH2CN to give Et 3-cyano-1,4-dihydro-5-methyl-4- oxopyrrolo[1,2-b]pyridazine-6-carboxylate.

This ketone was chlorinated and treated with cyclohexylamine to give the title compound II. The compds. I were tested against several different kinases such as VEGFR-2, FGFR-1, HER-1, HER-2, HER-4, MEK and p38 kinases. Thus, tested compds. I inhibited VEGFR-2 and FGFR-1 kinases with IC50 of ≤80 μM.

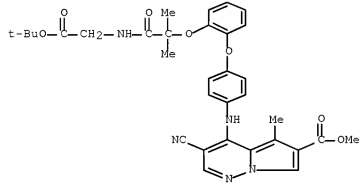
IT 779344-57-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of pyrrolopyridazines for the treatment of proliferative disorders)

RN 779344-57-9 HCAPLUS

CN Pyrrolo[1,2-b]pyridazine-6-carboxylic acid, 3-cyano-4-[[4-[2-[2-[[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]-1,1-dimethyl-2-oxoethoxy]phenoxy]phenyl]amino]-5-methyl-, methyl ester (CA INDEX NAME)



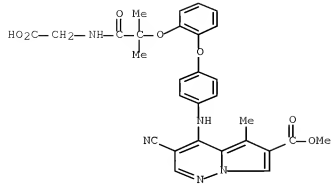
IT 779344-58-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrrolopyridazines for the treatment of proliferative disorders)

RN 779344-58-0 HCAPLUS

CN Pyrrolo[1,2-b]pyridazine-6-carboxylic acid, 4-[[4-[2-[2-[(carboxymethyl)amino]-1,1-dimethyl-2-oxoethoxy]phenoxy]phenyl]amino]-3-cyano-5-methyl-, 6-methyl ester (CA INDEX NAME)

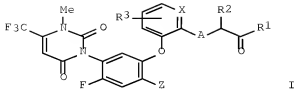


REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:946033 HCAPLUS Full-text
DOCUMENT NUMBER: 138:20910
TITLE: Preparation of 3-Methyl-2,6-dioxo-4-(trifluoromethyl)-1,2,3,6-tetrahydropyrimidine derivatives as plant growth regulators for cotton
INVENTOR(S): Mito, Nobuaki
PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan
SOURCE: PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002098227	A1	20021212	WO 2001-JP4584	20010531
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001262676	A1	20021216	AU 2001-262676	20010531
AU 2001262676	B2	20070125		
BR 2001017032	A	20040420	BR 2001-17032	20010531
US 20040152597	A1	20040805	US 2003-476511	20031103
US 7115544	B2	20061003		

PRIORITY APPLN. INFO.: WO 2001-JP4584 W 20010531
OTHER SOURCE(S): MARPAT 138:20910
GI



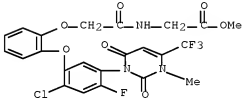
I

AB Plant growth regulators for cotton containing as an active ingredient a compound I (X = CH, or N; Z = halo; A = O, S, or NH; R1 = OH, C1-C7 alkoxy, C3-C7 alkenyloxy, C3-C7 alkynyloxy, C5-C7 cycloalkoxy, [di(C1-C7 alkoxy)carbonyl]C1-C3 alkoxy, (C1-C7 alkylamino)oxy, [di(C1-C7 alkyl)amino]oxy, (C3-C7 alkylideneamino)oxy, C1-C7 alkylamino, di(C1-C7 alkyl)amino, C3-C7 alkenylamino, C3-C7 alkynylamino, C5-C7 cycloalkylamino, [(C1-C7 alkoxy)carbonyl]C1-C3 alkylamino, or (C1-C7 alkoxy)amino; R2 = H, or Me; R3 = H, halo, C1-C3 alkyl, or C1-C3 alkoxy) are prepared

IT 380500-89-0P 477714-69-5P 477715-66-5P 477715-68-7P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as plant growth regulator for cotton)

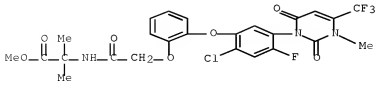
RN 380500-89-0 HCAPLUS

CN Glycine, N-[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



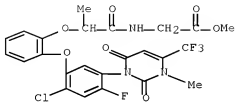
RN 477714-69-5 HCAPLUS

CN Alanine, N-[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

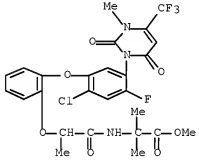


RN 477715-66-5 HCAPLUS

CN Glycine, N-[2-[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]-1-oxopropyl]-, methyl ester (CA INDEX NAME)



RN 477715-68-7 HCAPLUS
CN Alanine, N-[2-[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]-1-oxopropyl]-2-methyl-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:428894 HCAPLUS Full-text
DOCUMENT NUMBER: 137:20303
TITLE: Preparation of substituted quinolines as antitumor agents
INVENTOR(S): Boyle, Francis Thomas; Gibson, Keith Hopkinson; Foote, Kevin Michael
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044166	A1	20020606	WO 2001-GB4737	20011026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002010714	A	20020611	AU 2002-10714		20011026
EP 1337524	A1	20030827	EP 2001-978616		20011026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004514718	T	20040520	JP 2002-546536		20011026
US 20040029898	A1	20040212	US 2003-415812		20030502
US 7067532	B2	20060627			
US 20070021407	A1	20070125	US 2006-374423		20060314
US 7402583	B2	20080722			
PRIORITY APPLN. INFO.:			GB 2000-26744	A	20001102
			GB 2000-26746	A	20001102
			GB 2000-26747	A	20001102
			WO 2001-GB4737	W	20011026
			US 2003-415812	A3	20030502

OTHER SOURCE(S): MARPAT 137:20303
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

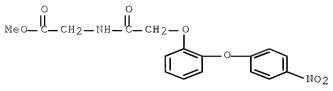
AB Title compds. I [n = 0 or 1; Y = NH, O, S, or alkylamine; R5 = CN, F, Cl, or Br; R6 = (un)substituted -cycloalkyl, -pyridinyl, -pyrimidinyl, -Ph, etc.; R1, R2 and R4 independently = H, OH, halo, CN, NO2, F3C, alkyl, amine, alkylamine, dialkylamine, R7X1(CH2)x- wherein x = 0-3, R7 = H, (un)substituted hydrocarbyl or heterocyclyl and X1 = O, CH2, OCO, CO, S, SO, SO2, NR8CO, NR8CO2, CONR9, CO2NR9, SO2NR10, NR11 or NR11NR11 wherein R8, R9, R10 and R11 independently = H, alkyl or alkoxyalkyl; R3 = group of formula X1R12(OH)p where p = 1-2 and R12 = alkylene, alkenylene or alkynylene chain, optionally interposed with a heteroatom or heterocyclic ring with the provision that when R12 = alkylene, R12 must be interposed with a heteroatom or heterocyclic ring and at least one (OH)p is on the alkylene chain between X1 and the interposed heteroatom or heterocyclic ring; group of formula R7(CH2)yX1(CH2)x where y = 0-5 and (CH2)y is optionally interposed by an X1 group; group of formula Xlalkyl where alkyl is substituted by one or more Cl and/or CN; heterocyclic ring, etc.], or a pharmaceutically acceptable salt, pro-drug or solvate thereof are prepared and disclosed as antiproliferative agents. Thus, II was prepared in eight steps from benzylchloroformate and 2-methoxy-5-nitroaniline. I were evaluated as inhibitors of MAPK pathway and exhibited IC50 values typically lest than 0.5 μM, e.g., II possessed an IC50 = 0.0013μM. In cell proliferation assays, I had IC50 results typically less than 30μM with II giving an IC50 of 1.3 μM in HT29 human colon tumor cells. Methods for prevention of cancer comprising administering an effective amount of compound I are further claimed.

IT 306999-95-1P 307309-82-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation, inhibition of MAP kinase, and cellular antiproliferation activity of substituted quinolines as antitumor agents)

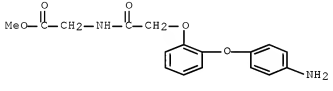
RN 306999-95-1 HCAPLUS

CN Glycine, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA

INDEX NAME)



RN 307309-82-6 HCAPLUS
CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:353433 HCAPLUS Full-text
DOCUMENT NUMBER: 136:369616
TITLE: Preparation of 3-cyano-4-arylaminoquinolines as inhibitors of MAP kinase for use as antitumor agents
INVENTOR(S): Boyle, Francis Thomas; Gibson, Keith Hopkinson
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 149 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002036570	A1	20020510	WO 2001-GB4733	20011025
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001095791	A	20020515	AU 2001-95791	20011025
EP 1337513	A1	20030827	EP 2001-976523	20011025

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2004517059	T	20040610	JP 2002-539330		20011025
US 20050101630	A1	20050512	US 2003-415813		20030502
US 7253184	B2	20070807			
US 20080027054	A1	20080131	US 2007-826507		20070716
US 7504416	B2	20090317			
PRIORITY APPLN. INFO.:			GB 2000-26745	A	20001102
			GB 2000-26747	A	20001102
			WO 2001-GB4733	W	20011025
			US 2003-415813	A3	20030502

OTHER SOURCE(S): MARPAT 136:369616
GI

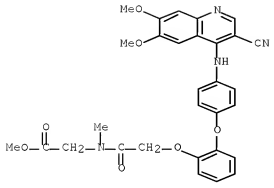
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1, R2, R3, R4 independently H, HO, halogen, NC, O2N, F3C, (un)substituted C1-C3 alkyl, (un)substituted amino, saturated heterocyclyl containing two heteroatoms; R5 = NC, F, Cl, Br; R6 = divalent C1-C5 alkenyl, C3-C7 cycloalkyl, or heteroaryl moiety; R7 = AR8; A = bond, O, CO, S, SO, SO2, (un)substituted aminocarbonyl, (un)substituted carbonylamino, (un)substituted sulfonylamino, (un)substituted aminosulfonyl, (un)substituted amino; R8 = C1-C6 alkyl, C2-C6 alkenyl, C2-C6 alkynyl; R9 = (un)substituted C3-C7 divalent cycloalkyl; R10 = (un)substituted arylene, heteroarylene, heteroarylene N-oxide, C3-C10 cycloalkylene; X = amino, (C1-C6)alkylamino, O, S, CH2; Y = amino, (C1-C6)alkylamino, O, S; Z = (un)substituted alkyl, alkylene, alkynylene, O, CO, COO, S, SO, SO2, (un)substituted aminocarbonyl, carbonylamino, sulfonylamino, aminosulfonyl, amino; n = 0,1; m and p independently 0-3; alternatively, R10Z(CH2)pR6R7 can be replaced with a heteroaryl or heterocyclyl-2,3-fused Ph ring] were prepared as inhibitors of MAP kinase for use as antitumor agents. E.g., 1-fluoro-4-nitrobenzene undergoes nucleophilic substitution with (2-hydroxyphenoxy)acetic acid followed by coupling of the acid with Me glycinate, reduction of the nitro group with Pd/C, and reaction of the ester with N-methylpiperazine to give the aminophenoxymethylcarbonylaminoacetyl piperazine II. E.g., coupling of II with 4-chloro-6,7-dimethoxy-3-quinolinenitrile gave the example compound III. Biol. data was obtained for selected compds. Selected compds. inhibited MAP kinase with IC50 < 0.5 μM; for example, III gave an IC50 of 3.8 nM. In addition, selected compds. inhibited the proliferation of human colon cancer cells with IC50 < 30 μM; for example, III gave an IC50 of 1 μM.

IT 423179-57-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(example compds.; preparation of 4-arylamino-3-cyanoquinolines as inhibitors of MAP kinase for potential use as antitumor agents)

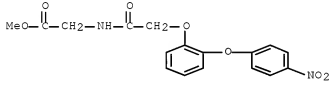
RN 423179-57-1 HCAPLUS

CN Glycine, N-[[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]acetyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

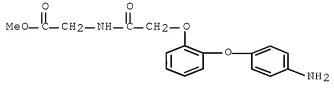


IT 306999-95-1P 307309-82-6P 423180-30-7P
423180-31-8P 423180-57-8P 423180-59-0P
423180-89-6P 423180-90-9P 423180-96-5P
423180-97-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediates; preparation of 4-arylamino-3-cyanoquinolines as inhibitors of MAP kinase for potential use as antitumor agents)

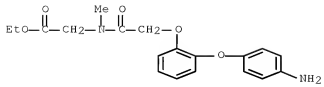
RN 306999-95-1 HCAPLUS
CN Glycine, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



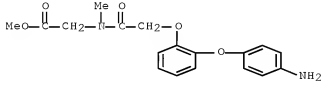
RN 307309-82-6 HCAPLUS
CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



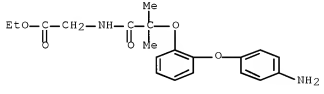
RN 423180-30-7 HCAPLUS
CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



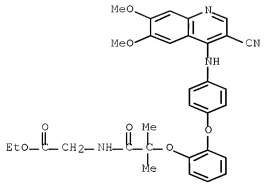
RN 423180-31-8 HCAPLUS
CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



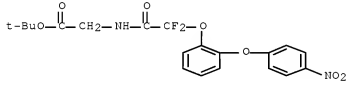
RN 423180-57-8 HCAPLUS
CN Glycine, N-[2-[2-(4-aminophenoxy)phenoxy]-2-methyl-1-oxopropyl]-, ethyl ester (CA INDEX NAME)



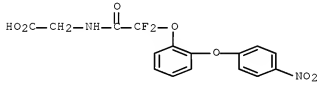
RN 423180-59-0 HCAPLUS
CN Glycine, N-[2-[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]-2-methyl-1-oxopropyl]-, ethyl ester (CA INDEX NAME)



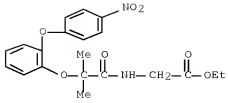
RN 423180-89-6 HCAPLUS
CN Glycine, N-[difluoro[2-(4-nitrophenoxy)phenoxy]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



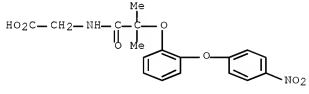
RN 423180-90-9 HCAPLUS
CN Glycine, N-[difluoro[2-(4-nitrophenoxy)phenoxy]acetyl]- (9CI) (CA INDEX NAME)



RN 423180-96-5 HCAPLUS
CN Glycine, N-[2-methyl-2-[2-(4-nitrophenoxy)phenoxy]-1-oxopropyl]-, ethyl ester (CA INDEX NAME)



RN 423180-97-6 HCAPLUS
CN Glycine, N-[2-methyl-2-[2-(4-nitrophenoxy)phenoxy]-1-oxopropyl]- (CA INDEX NAME)

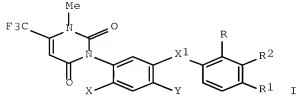


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:910259 HCAPLUS Full-text
DOCUMENT NUMBER: 136:53754
TITLE: Preparation and application of uracils as herbicides
INVENTOR(S): Goto, Tomohiko; Sanemitsu, Minoru
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 91 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001348376	A	20011218	JP 2000-170234	20000607
PRIORITY APPLN. INFO.:			JP 2000-170234	20000607

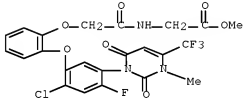
OTHER SOURCE(S): MARPAT 136:53754
GI



AB Title compds. [I; R = OCH(CH3)COOCH2COOCH3, (S)-OCH2CONHCH(CH2CH(CH3)2)CO2CH3, OCH2CONHCH2CO2CH3, OCH2CO2CH2CO2CH3, OCH2CO2C(CH3)2CO2CH2CH:CH2, H, CF3, CH3; R1 = H, OCH(CH3)CO2CH2COOH, OCH2COOCH2COOCH2CH:CH2, H; R2 = H, OCH(CH3)CO2CH2COOH, OCH2COOCH2COSCH2CH3; X = F, H; Y = Cl, NO2; X1 = O, S, NH] are prepared as herbicides. Thus, the title compound I (R = OCH2COOC(CH3)2COOCH2CH:CH2; R1 = H; R2 = H; X = F; X1 = O; Y = Cl) was prepared and field tested as effective herbicide in forage and soil treatment.

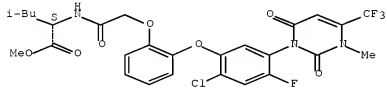
IT 380500-89-0P 380500-90-3P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and application of uracils as herbicides)

RN 380500-89-0 HCAPLUS
CN Glycine, N-[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 380500-90-3 HCAPLUS
CN L-Leucine, N-[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:814464 HCAPLUS Full-text
DOCUMENT NUMBER: 133:362712
TITLE: Preparation of quinoline derivatives as inhibitors of MEK enzymes
INVENTOR(S): Boyle, Francis Thomas; Gibson, Keith Hopkinson; Poyser, Jeffrey Philip; Turner, Paul
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 187 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068201	A1	20001116	WO 2000-GB1697	20000503
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2372663	A1	20001116	CA 2000-2372663	20000503
EP 1178967	A1	20020213	EP 2000-927491	20000503
EP 1178967	B1	20060308		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY				
TR 200103186	T2	20020422	TR 2001-3186	20000503
BR 2000010391	A	20020702	BR 2000-10391	20000503
HU 2002001219	A2	20020928	HU 2002-1219	20000503
HU 2002001219	A3	20030528		
EE 200100589	A	20030217	EE 2001-589	20000503
NZ 514980	A	20031031	NZ 2000-514980	20000503
AU 772846	B2	20040506	AU 2000-45891	20000503
CN 1219768	C	20050921	CN 2000-809959	20000503
EP 1584619	A1	20051012	EP 2005-13587	20000503
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, LV, FI, MK, CY, AL				
AT 319688	T	20060315	AT 2000-927491	20000503
PT 1178967	T	20060630	PT 2000-927491	20000503
ES 2258455	T3	20060901	ES 2000-927491	20000503
ZA 2001008971	A	20030130	ZA 2001-8971	20011030
IN 2001MN01338	A	20050304	IN 2001-MN1338	20011031
BG 106073	A	20020531	BG 2001-106073	20011101
NO 2001005448	A	20020107	NO 2001-5448	20011107
NO 321696	B1	20060626		
MX 2001011360	A	20020311	MX 2001-11360	20011107

PRIORITY APPLN. INFO.:	GB 1999-10577	A	19990508
	EP 2000-927491	A3	20000503
	WO 2000-GB1697	W	20000503

OTHER SOURCE(S): MARPAT 133:362712
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

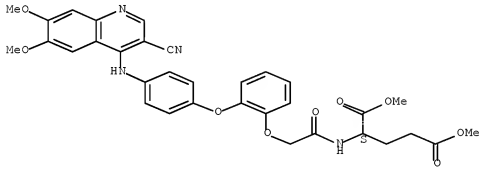
AB Title compds. [I; or a pharmaceutically acceptable salt thereof wherein: n is 0-1; X and Y are independently selected from NH, O, S, or NR8 where R8 is alkyl of 1-6 carbon atoms and X may addnl. comprise a CH2 group; R7 is a group (CH2)mR9 where m is 0, or an integer of from 1-3 and R9 is a substituted aryl group, an optionally substituted cycloalkyl ring of up to 10 carbon atoms, or an optionally substituted heterocyclic ring or an N-oxide of any nitrogen containing ring; R6 is a divalent cycloalkyl of 3 to 7 carbon atoms, which may

be optionally further substituted with one or more alkyl of 1 to 6 carbon atom groups; or is a divalent pyridinyl, pyrimidinyl, or Ph ring; wherein the pyridinyl, pyrimidinyl, or Ph ring may be optionally further substituted with one or more specified groups; R1, R2, R3 and R4 are each independently selected from hydrogen or various specified organic groups]. Title compds. are useful as pharmaceuticals for the inhibition of MEK activity. Thus, the title compound II was prepared and tested in HT29 human colon tumor cell proliferation assay.

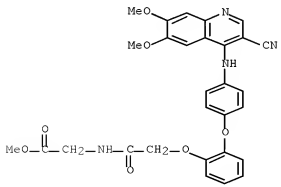
IT 306999-63-3P 306999-65-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of quinoline derivs. as inhibitors of MEK enzymes)

RN 306999-63-3 HCAPLUS
CN L-Glutamic acid, N-[[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]acetyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 306999-65-5 HCAPLUS
CN Glycine, N-[[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

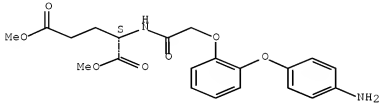


IT 306999-81-5 306999-85-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of quinoline derivs. as inhibitors of MEK enzymes)

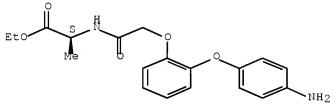
RN 306999-81-5 HCAPLUS
CN L-Glutamic acid, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 306999-85-9 HCAPLUS
CN L-Alanine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

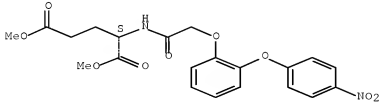
Absolute stereochemistry.



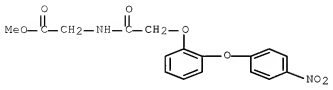
IT 306999-93-9P 306999-95-1P 306999-96-2P
307309-82-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinoline derivs. as inhibitors of MEK enzymes)

RN 306999-93-9 HCAPLUS
CN L-Glutamic acid, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

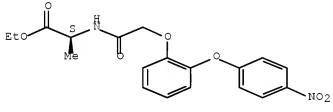


RN 306999-95-1 HCAPLUS
CN Glycine, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

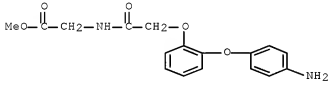


RN 306999-96-2 HCAPLUS
CN L-Alanine, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



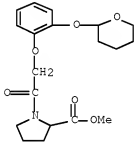
RN 307309-82-6 HCAPLUS
CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:64458 HCAPLUS Full-text
DOCUMENT NUMBER: 78:64458
ORIGINAL REFERENCE NO.: 78:10181a,10184a
TITLE: Detection of alkali metal ions by optical rotatory dispersion. Sensitive test for sodium in the presence of lithium and potassium
AUTHOR(S): Wudl, Fred
CORPORATE SOURCE: Dep. Chem., State Univ. N. Y., Buffalo, NY, USA

SOURCE: Journal of the Chemical Society, Chemical Communications (1972), (22), 1229-30
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The ORD curves of the chiral semicrown complexes (I, M = H, Li, Na, K) depend on the cation (M) and, as the interaction of I its strongest with Na, a spectropolarimetric determination of Na in the presence of Li and K is applicable.
IT 40418-12-0P
RL: PREP (Preparation)
(preparation of)
RN 40418-12-0 HCAPLUS
CN Proline, 1-[[2-[(tetrahydro-2H-pyran-2-yl)oxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



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=> d his nof

     (FILE 'HOME' ENTERED AT 12:47:29 ON 26 MAR 2009)

     FILE 'REGISTRY' ENTERED AT 12:47:46 ON 26 MAR 2009
L1                STRUCTURE UPLOADED
                  D
L2              0 SEA SSS SAM L1
L3                STRUCTURE UPLOADED
                  D
L4              0 SEA SSS SAM L3
L5                STRUCTURE UPLOADED
                  D
L6              0 SEA SSS SAM L5
L7                STRUCTURE UPLOADED
                   D

Uploading L3.str
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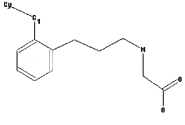
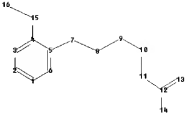


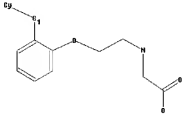


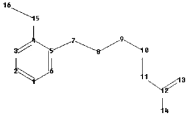
```
chain nodes :
7  12  13  14  15  16
ring nodes :
1  2  3  4  5  6
ring/chain nodes :
8  9  10  11
chain bonds :
4-15  5-7  7-8  11-12  12-13  12-14  15-16
ring/chain bonds :
8-9  9-10  10-11
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
4-15  8-9  9-10  10-11  12-13  12-14  15-16
exact bonds :
5-7  7-8  11-12
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 :


G1:O,S

Match level :
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

L8 0 SEA SSS SAM L7
L9 STRUCTURE UPLOADED
D

Uploading L5.str





chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

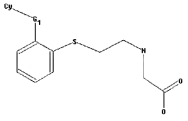
G1:O,S

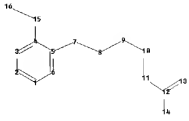
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:

Type of Ring System : Monocyclic

L10 1 SEA SSS SAM L9
L11 STRUCTURE UPLOADED

Uploading L6.str





chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

```
L12           0 SEA SSS SAM L11
L13           0 SEA SSS SAM L5 OR L9 OR L11
L14         171 SEA SSS FUL L5 OR L9 OR L11
                SAVE TEMP L14 BIA737REGCOM/A

     FILE 'HCAPLUS' ENTERED AT 13:11:11 ON 26 MAR 2009
L15          11 SEA ABB=ON  PLU=ON  L14
L16           1 SEA ABB=ON  PLU=ON  US20060235003/PN
L17       11570 SEA ABB=ON  PLU=ON  SMITH G?/AU
L18           6 SEA ABB=ON  PLU=ON  SMITH GARRICK/AU
L19          17 SEA ABB=ON  PLU=ON  MIKKELSEN G?/AU
L20          71 SEA ABB=ON  PLU=ON  ANDERSEN KIM/AU
L21         203 SEA ABB=ON  PLU=ON  GREVE D?/AU
L22          19 SEA ABB=ON  PLU=ON  ESKILDSEN J?/AU
L23           2 SEA ABB=ON  PLU=ON  (((L18 OR L19 OR L20 OR L21 OR L22)) AND
                L15) OR (L15 AND L16)
L24           9 SEA ABB=ON  PLU=ON  L15 NOT L23
                SAVE TEMP L23 BIA737HCAIN/A
                SAVE TEMP L24 BIA737HCAP/A
                D QUE L23
                D L23 1-2 IBIB ABS HITSTR
                D QUE L24
                D L24 1-9 IBIB ABS HITSTR
```